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Computational study of tungsten surface sputtering under various conditions

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Molecular Dynamics simulations is a powerful tool in investigating the effects on surfaces under various conditions. It is especially effective for studying the interaction between energetic particles and surfaces. Due to relevancy to fusion, tungsten surfaces have been studied under various conditions. Both pristine surfaces and atomistically rough surfaces have been studied under irradiation by various ion species and energies [1,2]. Simulations have in the last years revealed a plethora of insight into how different surface features will affect the sputtering and evolve under continuous irradiation [3,4]. It has been shown that the sputtering at high energies is directly related to the channeling in a certain direction of the incoming ion, which renders some of the simulation tools assuming amorphous materials questionable [5].

Another important factor under fusion conditions is the effect of hydrogen or its isotopes that are impacting the surface, causing sputtering, or get implantated into the surface layers. We have found that the sputtering by light elements, like hydrogen or its isotopes, is more complicated than previously thought. We found that the sputtering can happen due to several different mechanisms, which are not seen for heavier elements. We have also studied the effect of having the surface saturated with deuterium on the sputtering by both light and heavy ions. Again, we see that having a saturated surface versus a pristine one will affect the results.

All obtained results can be used as input in higher scale models in order to further predict their impact on material lifetimes and plasma properties.

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